



chain nodes :

13 14 15 16 17 18 19 20 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39
40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58

ring nodes :

1 2 3 4 5 6 7 8 9 10 11

chain bonds :

10-13 14-15 14-56 16-17 16-18 18-57 19-20 19-58 24-29 25-36 26-28 27-37 28-35
29-34 30-32 31-33 32-41 33-45 34-42 35-46 36-43 37-47 38-40 39-44 40-55 41-52
42-51 43-48 44-54 45-53 46-50 47-49

ring bonds :

1-2 1-7 2-3 2-8 3-4 3-11 4-5 5-6 6-7 8-9 9-10 10-11

exact/norm bonds :

1-2 1-7 2-3 2-8 3-4 3-11 4-5 5-6 6-7 8-9 9-10 10-11 10-13 14-15 16-18 28-35
29-34 30-32 31-33 33-45 35-46 37-47 39-44

exact bonds :

14-56 16-17 18-57 19-20 19-58 24-29 25-36 26-28 27-37 32-41 34-42 36-43 38-40
40-55 41-52 42-51 43-48 44-54 45-53 46-50 47-49

isolated ring systems :

containing 1 :

G1:X, [@1], [@2], [@3], [@4], [@5], [@6], [@7], [@8], [@9], [@10], [@11]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 24:CLASS
25:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS
34:CLASS 35:CLASS 36:CLASS 37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS
43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:Atom 49:Atom 50:Atom 51:Atom 52:Atom
53:Atom 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom